

Stochastic approach to correlations beyond the mean field with the Skyrme interaction

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Abstract. Large-scale calculation based on the multi-configuration Skyrme density functional theory is performed for the light $N = Z$ even-even nucleus, ^{12}C . Stochastic procedures and the imaginary-time evolution are utilized to prepare many Slater determinants. Each state is projected on eigenstates of parity and angular momentum. Then, performing the configuration mixing calculation with the Skyrme Hamiltonian, we obtain low-lying energy-eigenstates and their explicit wave functions. The generated wave functions are completely free from any assumption and symmetry restriction. Excitation spectra and transition probabilities are well reproduced, not only for the ground-state band, but for negative-parity excited states and the Hoyle state.

Keywords: NUCLEAR STRUCTURE, ^{12}C , Calculated levels, Configuration mixing. Skyrme interaction

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INTRODUCTION

Density functional theory is currently regarded as the only tractable theory that can be applied across the entire chart of nuclei. Since nuclei are self-bound systems, they produce their own effective confining potential (“mean field”). The mean field often leads to a symmetry-breaking state which represents certain correlation. However, for finite nuclei, quantitative description often requires the symmetry restoration and correlations beyond the mean field.

For light nuclei, it is important to take into account the cluster correlations, since a variety of cluster states are known to emerge in excited states at relatively low energy. Several theoretical approaches were developed for this [1], assuming cluster configurations, such as the resonating group method (RGM), the generator coordinate method (GCM), and the orthogonal condition model (OCM). In these approaches, the existence of clusters is assumed from the beginning.

Therefore, it is desirable to develop a method which is able to describe both full mean-field dynamics and correlations beyond mean field, including the cluster correlation, shape fluctuation, and shape mixing. For this purpose, in Ref. [2], we proposed a new approach and applied it to the simple BKN energy functional of Ref. [3]. The method is somewhat similar to the GCM, however, has an advantage over it. Namely, since we do not assume a generator coordinate (collective space) a priori, the calculation, in principle, may take account of all the possible correlations beyond the mean field. Its apparent drawback is necessity of heavy computational resources.

BRIEF DESCRIPTION OF METHOD

In this section, we briefly recapitulate our method. Readers should be referred to Ref.[2] for details.

We start with a Skyrme Hamiltonian, in the present work, with the SLy4 parameter set. Since the Skyrme interaction is an effective interaction with zero-range forces, it does not have a real (physical) ground state in the infinite Hilbert space. Thus, we must define the space consistent with the interaction.

For this purpose, we adopt stochastic generation and imaginary-time evolution of Slater determinants [2]. Initial Slater determinants are generated by using random numbers. However, these initial states contain high momentum components which are not consistent with the Skyrme interaction. This motivates us to use the imaginary-time method which can effectively remove these high-momentum components in the wave function. Thus, we simply discard Slater determinants produced by the imaginary-time propagation until the state is sufficiently cooled down.

The imaginary-time propagation produces a kind of “collective paths” which are associated with low-energy modes of excitation, eventually leads to the Hartree-Fock ground state. During this imaginary-time propagation, we regularly store the generated Slater determinants and check their linear independence according to a certain criterion [2]. The Slater determinants, $|\Phi_i\rangle$, are constructed in the mesh representation of the three-dimensional (3D) Cartesian coordinate space. Then, we perform the parity and the 3D angular-momentum projection, $|\Phi_i^{\pi IK}\rangle_M = P_{MK}^I |\Phi_i\rangle$. Finally we obtain the energy eigenstate, $|\Psi^{\pi I}\rangle = \sum_{iK} c_{iK}^{\pi I} |\Phi_i^{\pi IK}\rangle$, by solving the generalized eigenvalue equation in each parity and angular momentum sector:

$$\sum_{i'K'} \left(\mathcal{H}_{iK,i'K'}^{\pi I} - E \mathcal{N}_{iK,i'K'}^{\pi I} \right) c_{i'K'}^{\pi I} = 0. \quad (1)$$

Here, $\mathcal{H}_{iK,i'K'}^{\pi I}$ and $\mathcal{N}_{iK,i'K'}^{\pi I}$ are the Hamiltonian and norm kernels [4]. In order to avoid the overcompleteness problem in the configuration mixing calculation, if the smallest eigenvalue of the norm matrix $\mathcal{N}_{iK,i'K'}^{\pi I}$ is smaller than 10^{-3} , we reduce the number of basis.

The most time-consuming part of the calculation is the angular-momentum projection [5]. Since the wave functions are completely free from symmetry restriction, we must perform the full 3D rotation with respect to three Euler angles. This becomes more and more difficult as increasing the angular momentum. Because of this numerical difficulty, we only calculate low-spin states with $J < 6$. The most delicate part of the calculation is treatment of the overcomplete basis. This is discussed in detail in Ref. [2, 6].

RESULTS

We apply the method to calculation of excitation spectra in ^{12}C . The space is the sphere of the radius 8 fm which is discretized in mesh of $\Delta x = \Delta y = \Delta z = 0.8$ fm. In this paper, we show results with the SLy4 parameter set, however we confirm almost identical

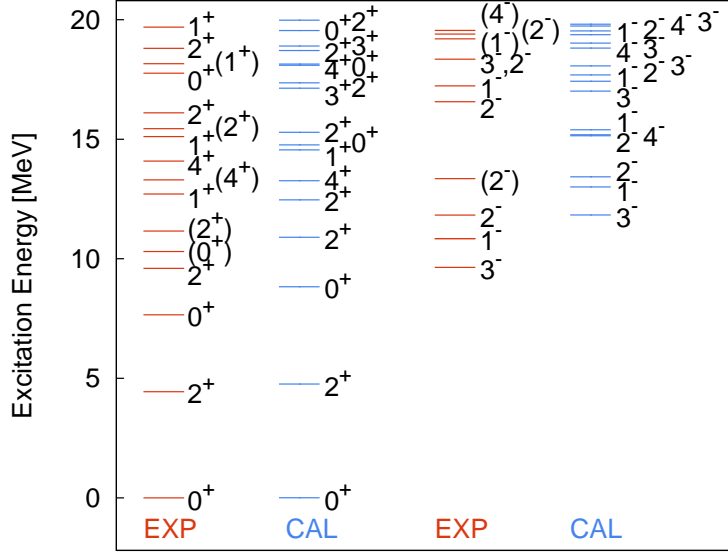


FIGURE 1. Excitation spectra in ^{12}C . The positive-parity and negative-parity states are shown in the left and right parts, respectively. The experimental data are taken from Refs. [7, 8, 9].

excitation spectra with the SkM*, SGII, and SIII parameters (although the absolute binding energy of the ground state is different).

In Fig. 1, we show the result. In the positive-parity sector, the calculation successfully produces the ground-state band ($J^\pi = 0^+, 2^+$, and 4^+ states). This rotational character comes from correlation beyond the mean field, because the Hartree-Fock ground state calculated with SLy4 parameter set has a spherical shape. $B(E2)$ transition strengths among these three states are calculated as $B(E2; 2_1^+ \rightarrow 0_1^+) = 8.6 \text{ e}^2\text{fm}^4$ and $B(E2; 4_1^+ \rightarrow 2_1^+) = 13.4 \text{ e}^2\text{fm}^4$. Experiments [7] indicate $B(E2; 2_1^+ \rightarrow 0_1^+) = 7.6 \pm 0.4 \text{ e}^2\text{fm}^2$ which is well reproduced in the present calculation.

The calculation also reproduces the second 0^+ state known as the Hoyle state, that plays a crucial role in the stellar Helium burning process. This state has recently been attracting attention as a condensed state of three-alpha particles [10]. In our calculation, this state is described as a superposition of many Slater determinants. However, the largest component actually exhibits an spatially extended structure of three alpha particles. The transition between the Hoyle state and the first 2^+ state was measured as $B(E2; 0_2^+ \rightarrow 2_1^+) = 13 \pm 2 \text{ e}^2\text{fm}^4$. The calculated value is $13.6 \text{ e}^2\text{fm}^4$ in good agreement with the experiment. The calculation also well reproduces the $E0$ transition matrix element between the ground state and Hoyle state; $M(E0)_{\text{cal}} = 4.5 \text{ fm}^2$ for the experimental value, $M(E0)_{\text{exp}} = 5.4 \pm 0.2 \text{ fm}^2$.

The calculated third 0^+ state at $E_x \approx 15 \text{ MeV}$ has a very elongated structure, which may be regarded as a linear chain of the three alpha's. This state has a large $B(E2)$ transition strength to 2_4^+ state.

Negative-parity states are also reasonably well reproduced in the calculation, though the excitation energy is too high by a few MeV. We obtain the correct ordering among

different J multiplets. It turns out that major components of the low-lying negative parity states (3_1^- , 1_1^- , and 2_1^- states) are the three-alpha structure, but their spatial extension is smaller than that of the 0_2^+ state.

CONCLUSION

We have performed the 3D real-space calculations of the multi-configuration Skyrme density functional theory, using the stochastic generation and the imaginary-time propagation of Slater determinants. We solve the generalized eigenvalue problem in a generated model space after the parity and angular-momentum projection. Low-lying spectra in ^{12}C are well reproduced. Properties of the ground-state band, which consists of 0_1^+ , 2_1^+ , and 4_1^+ states, are almost perfectly reproduced. The Hoyle state (0_2^+ state) also shows a nice agreement with experiment. It is known that the Hoyle state cannot be described in a small model space, because of its spatially extended character. The satisfactory description of the Hoyle state indicates that the present approach in the 3D coordinate-space representation is able to take into account correlations beyond the mean field in a very large model space.

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